

# Time-dependent multi-orbital mean-field for fragmented Bose-Einstein condensates

O. E. Alon\*, A. I. Streltsov<sup>†</sup>, and L. S. Cederbaum<sup>‡</sup>

*Theoretische Chemie, Physikalisch-Chemisches Institut, Universität Heidelberg,  
Im Neuenheimer Feld 229, D-69120 Heidelberg, Germany*

## Abstract

The evolution of Bose-Einstein condensates is usually described by the famous time-dependent Gross-Pitaevskii equation, which assumes all bosons to reside in a single time-dependent orbital. In the present work we address the evolution of fragmented condensates, for which two (or more) orbitals are occupied, and derive a corresponding time-dependent multi-orbital mean-field theory. We call our theory TDMF( $n$ ), where  $n$  stands for the number of evolving fragments. Working equations for a general two-body interaction between the bosons are explicitly presented along with an illustrative numerical example.

Typeset using REVTeX

---

\*E-mail: ofir@tc.pci.uni-heidelberg.de

<sup>†</sup>E-mail: alexej@tc.pci.uni-heidelberg.de

<sup>‡</sup>E-mail: lorenz.cederbaum@pci.uni-heidelberg.de

## I. INTRODUCTION

The properties and evolution of Bose-Einstein condensates have been extensively explored in the community by employing the famous time-independent and time-dependent Gross-Pitaevskii equation, for reviews see [1,2] and for individual applications, e.g., Refs. [3–9].

Gross-Pitaevskii theory is an excellent mean-field for weakly-interacting bosons whenever a single macroscopic one-particle wavefunction is sufficient to describe the reality. By definition, Gross-Pitaevskii theory cannot describe fragmentation of condensates for which two (or more) one-particle wavefunctions are macroscopically occupied. Recently, we have developed a time-independent multi-orbital mean-field to describe static properties of condensates [10,11], thus generalizing the (one-orbital) Gross-Pitaevskii mean-field. For other approaches to fragmentation of Bose-Einstein condensates, see, e.g., Refs. [12–14]. Utilizing the multi-orbital mean-field has enabled us to find new phenomena associated with fragmentation as well as fermionization of bosonic atoms in traps and optical lattices [15–18]. Motivated by this wealth of phenomena in the stationary case, it is the purpose of this work to derive a *time-dependent* multi-orbital mean-field theory, thus generalizing the *time-dependent* Gross-Pitaevskii equation. This will enable one to study dynamical properties of fragmented condensates evolving in time.

## II. PRELIMINARIES: TIME-DEPENDENT GROSS-PITAEVSKII EQUATION FROM VARIATIONAL PRINCIPLE

The evolution of  $N$  interacting structureless bosons is governed by the time-dependent Schrödinger equation:

$$\hat{H}\Phi = i\frac{\partial\Phi}{\partial t}, \quad \hat{H}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \sum_{i=1}^N \hat{h}(\mathbf{r}_i) + \sum_{i>j=1}^N \lambda_0 V(\mathbf{r}_i - \mathbf{r}_j). \quad (1)$$

Here  $\hbar = 1$ ,  $\mathbf{r}_i$  is the coordinate of the  $i$ -th boson,  $\hat{h}(\mathbf{r})$  is the one-body Hamiltonian containing kinetic and potential energy terms, and  $\lambda_0 V(\mathbf{r}_i - \mathbf{r}_j)$  describes the pairwise interaction

between the  $i$ -th and  $j$ -th atoms where  $\lambda_0$  measures the strength of the interparticle interaction.

The time-dependent Schrödinger equation (1) cannot be solved analytically, except for a few specific cases only. Thus, approximations are a must. The standard (and simplest) mean-field approximation to the time-dependent many-body wavefunction  $\Phi$  assumes all bosons to reside in a single *time-dependent* orbital  $\phi(\mathbf{r}, t)$ , namely, that the many-body wavefunction is written as

$$\Phi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N, t) = \phi(\mathbf{r}_1, t)\phi(\mathbf{r}_2, t) \cdots \phi(\mathbf{r}_N, t). \quad (2)$$

This so-called Hartree approximation, as is well known, gives rise to the famous time-dependent Gross-Pitaevskii equation [1,2]. For our needs, it would be instructive to show how the time-dependent Gross-Pitaevskii equation derives from a variational principle. To this end we employ the usual functional action, see, e.g., Refs. [19,20], which reads:

$$S = \int dt \left\{ \left\langle \Phi \left| \hat{H} - i \frac{\partial}{\partial t} \right| \Phi \right\rangle - \mu(t) [\langle \phi | \phi \rangle - 1] \right\}, \quad (3)$$

where the time-dependent Lagrange multiplier  $\mu(t)$  is introduced to ensure that  $\phi(\mathbf{r}, t)$  remains normalized throughout the propagation. To evaluate this action we use the ansatz (2) and find:

$$\begin{aligned} \left\langle \Phi \left| \hat{H} - i \frac{\partial}{\partial t} \right| \Phi \right\rangle &= N \int \phi^*(\mathbf{r}, t) \left[ \hat{h}(\mathbf{r}) - i \frac{\partial}{\partial t} \right] \phi(\mathbf{r}, t) d\mathbf{r} + \\ &+ \lambda_0 \frac{N(N-1)}{2} \iint \phi^*(\mathbf{r}, t) \phi^*(\mathbf{r}', t) V(\mathbf{r} - \mathbf{r}') \phi(\mathbf{r}, t) \phi(\mathbf{r}', t) d\mathbf{r} d\mathbf{r}'. \end{aligned} \quad (4)$$

By requiring stationarity of the action with respect to variation of  $\phi^*(\mathbf{r}, t)$ , namely,  $\frac{\delta S}{\delta \phi^*(\mathbf{r}, t)} = 0$ , we readily obtain the equation of motion:

$$N \left[ \hat{h}(\mathbf{r}) + \lambda_0(N-1) \hat{J}(\mathbf{r}, t) \right] \phi(\mathbf{r}, t) = iN \dot{\phi}(\mathbf{r}, t) + \mu(t) \phi(\mathbf{r}, t), \quad (5)$$

where the direct, time-dependent local potential  $\hat{J}(\mathbf{r}, t)$  reads

$$\hat{J}(\mathbf{r}, t) = \int \phi^*(\mathbf{r}', t) V(\mathbf{r} - \mathbf{r}') \phi(\mathbf{r}', t) d\mathbf{r}', \quad (6)$$

and the shorthand notation  $\dot{\phi} \equiv \frac{\partial \phi}{\partial t}$  has been introduced.

Using the constraint that  $\phi(\mathbf{r}, t)$  is normalized we can eliminate the Lagrange multiplier  $\mu(t)$  from Eq. (5). By taking the scalar product of  $\phi^*(\mathbf{r}, t)$  with (5), the resulting  $\mu(t)$  takes on the form,

$$\mu(t) = N \int \phi^*(\mathbf{r}, t) \left[ \hat{h}(\mathbf{r}) - i \frac{\partial}{\partial t} + \lambda_0(N-1) \hat{J}(\mathbf{r}, t) \right] \phi(\mathbf{r}, t) d\mathbf{r}. \quad (7)$$

Substituting Eq. (7) into Eq. (5) and noticing the identity

$$\begin{aligned} & \left[ \hat{h}(\mathbf{r}) - i \frac{\partial}{\partial t} + \lambda_0(N-1) \hat{J}(\mathbf{r}, t) \right] \phi(\mathbf{r}, t) - \frac{\mu(t)}{N} \phi(\mathbf{r}, t) = \\ & = \left( 1 - \phi(\mathbf{r}, t) \int \phi^*(\mathbf{r}, t) d\mathbf{r} \right) \left[ \hat{h}(\mathbf{r}) - i \frac{\partial}{\partial t} + \lambda_0(N-1) \hat{J}(\mathbf{r}, t) \right] \phi(\mathbf{r}, t), \end{aligned} \quad (8)$$

we arrive immediately at the time-dependent mean-field equation:

$$\begin{aligned} \mathbf{P} i \dot{\phi}(\mathbf{r}, t) &= \mathbf{P} \left[ \hat{h}(\mathbf{r}) + \lambda_0(N-1) \hat{J}(\mathbf{r}, t) \right] \phi(\mathbf{r}, t), \\ \mathbf{P} &= 1 - \phi(\mathbf{r}, t) \int \phi^*(\mathbf{r}, t) d\mathbf{r}. \end{aligned} \quad (9)$$

Examining Eq. (9) we see that eliminating the Lagrange multiplier  $\mu(t)$  has emerged as a projection operator  $\mathbf{P}$  onto the subspace spanned by  $\phi(\mathbf{r}, t)$ . This projection appears both on the left- and right-hand-sides of (9), making it a somewhat cumbersome integro-differential non-linear equation. To simplify its appearance we choose the relation

$$\int \phi^*(\mathbf{r}, t) \dot{\phi}(\mathbf{r}, t) d\mathbf{r} = 0 \quad (10)$$

at any time. This condition is equivalent to making the assignment of the time-dependent phase  $\phi(\mathbf{r}, t) \rightarrow \exp \left\{ + \int \langle \phi | \dot{\phi} \rangle dt \right\} \phi(\mathbf{r}, t)$  in Eq. (9). With this condition, the influence of the projection on the left-hand-side simplifies,  $\mathbf{P} \dot{\phi}(\mathbf{r}, t) = \dot{\phi}(\mathbf{r}, t)$ , and (9) takes on the appealing form:

$$\begin{aligned} i \dot{\phi}(\mathbf{r}, t) &= \mathbf{P} \left[ \hat{h}(\mathbf{r}) + \lambda_0(N-1) \hat{J}(\mathbf{r}, t) \right] \phi(\mathbf{r}, t), \\ \mathbf{P} &= 1 - \phi(\mathbf{r}, t) \int \phi^*(\mathbf{r}, t) d\mathbf{r}. \end{aligned} \quad (11)$$

The  $\mathbf{P}$  remaining on the right-hand-side of Eq. (11) makes it clear that the condition (10) is indeed satisfied at any time throughout the propagation of  $\phi(\mathbf{r}, t)$ . In practice, the meaning of this condition is that the temporal change of  $\phi(\mathbf{r}, t)$  is always orthogonal to  $\phi(\mathbf{r}, t)$  itself, which can be exploited to maintain accurate propagation results at lower computational costs. Additionally with condition (10),  $\mu(t)$  in Eq. (7) takes now an appealing form which can be interpreted as ( $N$  times) the time-dependent chemical potential of the condensate.

To complete this section we would like to show that the three equations, Eq. (9), Eq. (11) and the equation obtained by 'omitting' the projector  $\mathbf{P}$  completely are fully equivalent to each other. To this end, we notice that the Lagrange multiplier  $\mu(t)$  can be 'absorbed' into  $\phi(\mathbf{r}, t)$  by making the assignment  $\phi(\mathbf{r}, t) \rightarrow \exp \{i/N \int \mu(t) dt\} \phi(\mathbf{r}, t)$ . This immediately results in the time-dependent Hartree mean-field equation

$$i\dot{\phi}(\mathbf{r}, t) = [\hat{h}(\mathbf{r}) + \lambda_0(N-1)\hat{J}(\mathbf{r}, t)] \phi(\mathbf{r}, t). \quad (12)$$

In other words, in the case of a single orbital  $\phi$ , one can either use the form (9), the form (11) or the form (12).

Finally, to arrive at the time-dependent Gross-Pitaevskii equation in its usual appearance we take  $\lambda_0 V(\mathbf{r} - \mathbf{r}') = \lambda_0 \delta(\mathbf{r} - \mathbf{r}')$  and set  $\lambda_0$  proportional to the s-wave scattering length in any of the above equivalent forms (9), (11) or (12). Consequently, the direct potential (6) simplifies,  $\hat{J}(\mathbf{r}, t) = |\phi(\mathbf{r}, t)|^2$ , leading to the familiar result [1,2]:

$$i\dot{\phi}(\mathbf{r}, t) = [\hat{h}(\mathbf{r}) + \lambda_0(N-1)|\phi(\mathbf{r}, t)|^2] \phi(\mathbf{r}, t). \quad (13)$$

In what follows we generalize the time-dependent Gross-Pitaevskii equation, which is only valid for non-fragmented condensates, by constructing a multi-orbital time-dependent mean-field for fragmented condensates. We will generalize the forms (9) and (11) of the time-dependent Gross-Pitaevskii equation where in the latter case constraints such as (10) would make the interpretation of the results as well as the numerical implementation particularly useful.

### III. TIME-DEPENDENT MULTI-ORBITAL MEAN-FIELD EQUATIONS FOR BOSONS

Generalizing the stationary multi-orbital mean-field ansatz [10,11], the most general time-dependent mean-field *wavefunction* for  $N$  interacting bosons is the *single* configuration time-dependent wavefunction

$$\Phi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N, t) = \hat{\mathcal{S}}\phi_1(\mathbf{r}_1, t)\phi_2(\mathbf{r}_2, t) \cdots \phi_N(\mathbf{r}_N, t), \quad (14)$$

where  $\hat{\mathcal{S}}$  is the symmetrization operator. Of course, for bosons not all  $\phi_k(\mathbf{r}, t)$  have to be different functions. For instance, in the Hartree (or Gross-Pitaevskii) ansatz (2) all  $\phi_k(\mathbf{r}, t)$  are taken to be equal to one another. Generally, however, we may take  $n_1$  bosons to reside in  $\phi_1(\mathbf{r}, t)$ ,  $n_2$  bosons to reside in a different orbital  $\phi_2(\mathbf{r}, t)$ , and so on, as long as the set of occupations  $\{n_k\}$  satisfies  $n_1 + n_2 + \dots + n_{orb} = N$  and, of course, the number  $n_{orb}$  of different orbitals satisfies  $1 \leq n_{orb} \leq N$ . What is important to note is that the different orbitals  $\phi_k(\mathbf{r}, t)$  within ansatz (14) are propagated variationally in time and remain *normalized* and *orthogonal* to one another at any time.

To proceed for any set of  $n_{orb}$  orbitals and a corresponding set of occupations  $\{n_k\}$ , we substitute the ansatz (14) for  $\Phi$  into the usual functional action which now reads:

$$S = \int dt \left\{ \left\langle \Phi \left| \hat{H} - i \frac{\partial}{\partial t} \right| \Phi \right\rangle - \sum_{k,j}^{n_{orb}} \mu_{kj}(t) [\langle \phi_k | \phi_j \rangle - \delta_{kj}] \right\}, \quad (15)$$

where the time-dependent Lagrange multipliers  $\mu_{kj}(t)$  are introduced to ensure that the time-dependent orbitals  $\phi_k(\mathbf{r}, t)$  remain orthonormal throughout the propagation. The expectation value in the action takes on the appearance

$$\begin{aligned} \left\langle \Phi \left| \hat{H} - i \frac{\partial}{\partial t} \right| \Phi \right\rangle &= \\ &= \sum_k^{n_{orb}} n_k \left[ h_{kk} - \left( i \frac{\partial}{\partial t} \right)_{kk} + \lambda_0 \frac{n_k - 1}{2} V_{kkkk} + \frac{1}{2} \sum_{l \neq k}^{n_{orb}} \lambda_0 n_l V_{kl[kl]} \right], \end{aligned} \quad (16)$$

where the one- and two-body matrix elements are given by

$$\begin{aligned}
h_{kj} &= \int \phi_k^*(\mathbf{r}) h(\mathbf{r}) \phi_j(\mathbf{r}) d\mathbf{r}, \\
\left(i \frac{\partial}{\partial t}\right)_{kj} &= i \int \phi_k^*(\mathbf{r}) \dot{\phi}_j(\mathbf{r}) d\mathbf{r}, \\
V_{kjql} &= \iint \phi_k^*(\mathbf{r}) \phi_j^*(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \phi_q(\mathbf{r}) \phi_l(\mathbf{r}') d\mathbf{r} d\mathbf{r}', \\
V_{kj[ql]} &= V_{kjql} + V_{kj lq}.
\end{aligned} \tag{17}$$

Note the plus sign in  $V_{kj[ql]}$  which is due to the symmetrization operator.

By requiring stationarity of the action with respect to variation of all  $\phi_k^*(\mathbf{r}, t)$ , namely,  $\frac{\delta S}{\delta \phi_k^*(\mathbf{r}, t)} = 0, k = 1, \dots, n_{orb}$ , we obtain a set of  $n_{orb}$  equations of motion for the multi-orbital mean-field ansatz (14):

$$\begin{aligned}
n_k \left[ \hat{h} - i \frac{\partial}{\partial t} + \lambda_0(n_k - 1) \hat{J}_k + \sum_{l \neq k}^{n_{orb}} \lambda_0 n_l (\hat{J}_l + \hat{K}_l) \right] |\phi_k\rangle = \\
= \sum_j^{n_{orb}} \mu_{kj}(t) |\phi_j\rangle, \quad k = 1, \dots, n_{orb},
\end{aligned} \tag{18}$$

where the direct (local) and exchange (non-local) time-dependent potentials are given by

$$\begin{aligned}
\hat{J}_l(\mathbf{r}, t) &= \int \phi_l^*(\mathbf{r}', t) V(\mathbf{r} - \mathbf{r}') \phi_l(\mathbf{r}', t) d\mathbf{r}', \\
\hat{K}_l(\mathbf{r}, t) &= \int \phi_l^*(\mathbf{r}', t) V(\mathbf{r} - \mathbf{r}') \mathcal{P}_{\mathbf{r}\mathbf{r}'} \phi_l(\mathbf{r}', t) d\mathbf{r}',
\end{aligned} \tag{19}$$

and  $\mathcal{P}_{\mathbf{r}\mathbf{r}'}$  permutes the  $\mathbf{r}$  and  $\mathbf{r}'$  coordinates of two bosons appearing to the right of it.

Using the constraints that the  $\phi_k(\mathbf{r}, t)$  are orthonormal functions we can eliminate the Lagrange multipliers  $\mu_{kj}(t)$  from Eq. (18). By taking the scalar product of  $\langle \phi_j |$  with (18), the resulting  $\mu_{kj}(t)$  take on the form,

$$\mu_{kj}(t) = n_k \left[ h_{jk} - \left(i \frac{\partial}{\partial t}\right)_{jk} + \lambda_0(n_k - 1) V_{jkkk} + \sum_{l \neq k}^{n_{orb}} \lambda_0 n_l V_{jl[kl]} \right]. \tag{20}$$

Substituting Eq. (20) into Eq. (18) and noticing the identities

$$\begin{aligned}
\left[ \hat{h} - i \frac{\partial}{\partial t} + \lambda_0(n_k - 1) \hat{J}_k + \sum_{l \neq k}^{n_{orb}} \lambda_0 n_l (\hat{J}_l + \hat{K}_l) \right] |\phi_k\rangle - \frac{1}{n_k} \sum_j^{n_{orb}} \mu_{kj}(t) |\phi_j\rangle = \\
\left( 1 - \sum_{j=1}^{n_{orb}} |\phi_j\rangle \langle \phi_j| \right) \left[ \hat{h} - i \frac{\partial}{\partial t} + \lambda_0(n_k - 1) \hat{J}_k + \sum_{l \neq k}^{n_{orb}} \lambda_0 n_l (\hat{J}_l + \hat{K}_l) \right] |\phi_k\rangle
\end{aligned} \tag{21}$$

for all  $k$ , we arrive immediately at the time-dependent multi-orbital mean-field equations,  $k = 1, \dots, n_{orb}$ :

$$\begin{aligned} \mathbf{P}i|\dot{\phi}_k\rangle &= \mathbf{P} \left[ \hat{h} + \lambda_0(n_k - 1)\hat{J}_k + \sum_{l \neq k}^{n_{orb}} \lambda_0 n_l (\hat{J}_l + \hat{K}_l) \right] |\phi_k\rangle, \\ \mathbf{P} &= 1 - \sum_{j=1}^{n_{orb}} |\phi_j\rangle\langle\phi_j|. \end{aligned} \quad (22)$$

Examining Eq. (22) we see that eliminating the Lagrange multipliers  $\mu_{kj}(t)$  has emerged as a projection operator  $\mathbf{P}$  onto the subspace spanned by the  $\phi_k(\mathbf{r}, t)$ . This projection appears both on the left- and right-hand-sides of (22), making it a coupled system of integro-differential non-linear equations.

The equation set (22) is the time-dependent multi-orbital mean-field which generalizes the one-orbital time-dependent mean-field equation (9). We call our theory in short TDMF( $n$ ), where  $n = n_{orb}$  stands for the number of evolving fragments. Similarly to the stationary case [10,11], the multi-orbital time-dependent theory boils down to the standard time-dependent mean-field for  $n_{orb} = 1$ . In contrast to the stationary case, where the occupations  $n_k$  of the fragments are also determined variationally, the  $n_k$  are determined by the initial condition, say at  $t = 0$ , and remain unaltered during the propagation. To enable the variation of the occupations in time, a much more involved many-body theory is needed. Such a theory is possible [21].

The multi-orbital coupled system (22) is more involved than its one-orbital predecessor Eq. (9). Naturally and similarly to the previous section, we would like to make its appearance simpler. We can choose the relations

$$\langle\phi_k|\dot{\phi}_k\rangle = 0, \quad k = 1, \dots, n_{orb} \quad (23)$$

at any time, which is equivalent to making the assignments of the time-dependent phases  $\phi_k(\mathbf{r}, t) \rightarrow \exp \left\{ + \int \langle\phi_k|\dot{\phi}_k\rangle dt \right\} \phi_k(\mathbf{r}, t)$  in Eq. (22). With these conditions, the influence of the projectors on the left-hand-side slightly simplifies,  $\mathbf{P}|\dot{\phi}_k\rangle = \mathbf{P}_k|\dot{\phi}_k\rangle$ , where  $\mathbf{P}_k = 1 - \sum_{j \neq k}^{n_{orb}} |\phi_j\rangle\langle\phi_j|$ . Additionally, the diagonal Lagrange multiplier  $\mu_{kk}(t)$ , see Eq. (20), can now be interpreted as ( $n_k$  times) the time-dependent chemical potential of the  $k$ -th fragment,



thus generalizing the time-independent quantities [10,16]. However, since the off-diagonal terms  $\langle \phi_k | \dot{\phi}_j \rangle, k \neq j$  can *a priori* not be absorbed in a similar manner by time-dependent phases, the system of coupled TDMF( $n$ ) equations, combining Eqs. (22) and (23), remains involved.

To proceed let us examine a few properties of the time-dependent multi-orbital mean-field for bosons, TDMF( $n$ ). First, it is clear that an initially normalized permanent  $\Phi$  remains normalized throughout the propagation since the orbitals  $\phi_k(\mathbf{r}, t)$  remain orthonormal functions at any time. Second, the expectation value of the Hamiltonian with respect to  $\Phi$  should be constant if the many-body Hamiltonian  $\hat{H}$  is time-independent. To examine this, we calculate the time derivative of  $\langle \Phi | \hat{H} | \Phi \rangle$ . Taking the scalar product of  $\dot{\phi}_k(\mathbf{r}, t)$  with Eq. (18), summing up over  $k$  and adding the result to its complex conjugate we readily obtain:

$$\begin{aligned} \frac{d}{dt} \langle \Phi | \hat{H} | \Phi \rangle &= \sum_k^{n_{orb}} n_k \left[ h_{\dot{k}k} + h_{k\dot{k}} + \lambda_0(n_k - 1) (V_{k\dot{k}kk} + V_{k\dot{k}kk}) + \right. \\ &\quad \left. + \sum_{l \neq k}^{n_{orb}} \lambda_0 n_l (V_{\dot{k}l[kl]} + V_{kl[\dot{k}l]}) \right] = \\ &= \sum_{k,j}^{n_{orb}} \left[ \mu_{kj}(t) \langle \dot{\phi}_k | \phi_j \rangle + \mu_{jk}^*(t) \langle \phi_k | \dot{\phi}_j \rangle \right]. \end{aligned} \quad (24)$$

In (24) we use the shorthand notation for the index  $\dot{k}$  to indicate expectation values with respect to  $\dot{\phi}_k(\mathbf{r}, t)$ , e.g.,  $h_{\dot{k}k} = \langle \dot{\phi}_k | \hat{h} | \phi_k \rangle$ , etc. From Eq. (24) we see that the energy would be conserved if the matrix of Lagrange multiplier is Hermitian,  $\mu_{kj}(t) = \mu_{jk}^*(t)$ , simply because

$$\langle \dot{\phi}_k | \phi_j \rangle + \langle \phi_k | \dot{\phi}_j \rangle = 0, \quad k, j = 1, \dots, n_{orb} \quad (25)$$

hold due to the orthonormality constraints. Whether throughout the time propagation of Eq. (22) the matrix of Lagrange multipliers  $\mu_{kj}(t)$  can be kept Hermitian at all times is a matter of further studies. There is an alternative to this Hermiticity condition, in the form of solutions to Eq. (22) which obey the constraints [22]

$$\langle \phi_k | \dot{\phi}_j \rangle = 0, \quad k, j = 1, \dots, n_{orb} \quad (26)$$

at any time. When these additional constraints are explicitly invoked, the energy is readily conserved, see Eq. (24). The influence of the projection on  $|\dot{\phi}_k\rangle$  simplifies considerably,  $\mathbf{P}|\dot{\phi}_k\rangle = |\dot{\phi}_k\rangle$ , and thus (22) takes on the appealing form,  $k = 1, \dots, n_{orb}$ :

$$i|\dot{\phi}_k\rangle = \mathbf{P} \left[ \hat{h} + \lambda_0(n_k - 1)\hat{J}_k + \sum_{l \neq k}^{n_{orb}} \lambda_0 n_l (\hat{J}_l + \hat{K}_l) \right] |\phi_k\rangle, \\ \mathbf{P} = \left( 1 - \sum_{j=1}^{n_{orb}} |\phi_j\rangle\langle\phi_j| \right). \quad (27)$$

The  $\mathbf{P}$  remaining on the right-hand-side of Eq. (27) makes it clear that the constraints (26) are indeed satisfied at any time throughout the propagation of  $\phi_k(\mathbf{r}, t)$ . In practice, the meaning of these constraints is that the temporal changes of the  $\phi_k(\mathbf{r}, t)$  are always orthogonal to the  $\phi_k(\mathbf{r}, t)$  themselves, a property which makes the time propagation of Eq. (27) robust and stable and which can thus be exploited to maintain accurate propagation results at lower computational costs.

To complete our derivation we would like to pose the question whether, similarly to the property of the time-dependent Hartree mean-field discussed in the previous section, see Eq. (12), the projector  $\mathbf{P}$  may totally be 'omitted' in the TDMF( $n$ ) theory. Examining Eq. (18) we note that the diagonal Lagrange multipliers  $\mu_{kk}(t)$  can indeed be 'absorbed' into the orbitals  $\phi_k(\mathbf{r}, t)$  by making the assignments  $\phi_k(\mathbf{r}, t) \rightarrow \exp \{i/n_k \int \mu_{kk}(t) dt\} \phi_k(\mathbf{r}, t)$ . However, in contrast to this situation the off diagonal Lagrange multipliers  $\mu_{kj}(t)$ ,  $k \neq j$ , which ensures orthogonality of the orbitals at any time, cannot in general be 'absorbed' into the evolution of the  $\phi_k(\mathbf{r}, t)$ , namely that the form (12) does not generally exist in the TDMF( $n$ ) theory. Therefore and in view of all the above, it is the version (27) of the TDMF( $n$ ) which will be implemented and employed below in our numerical example.

Finally, we mention that the presently developed time-dependent multi-orbital theory and its stationary version are intimately connected via the so-called imaginary-time propagation technique. It is well known that the ground state of the stationary Gross-Pitaevskii equation can be obtained by propagating in imaginary time the time-dependent Gross-Pitaevskii equation, see, e.g., [7]. In our case, by setting  $t \rightarrow -it$ , the left-hand-sides of (22)

and (27) decay to zero in time. Then, by using the identity (21) and the expression (20) for the Lagrange multipliers, the right-hand-sides of (22) and (27) boil down to the stationary multi-orbital mean-field theory [10,11]. This establishes a natural connection between the time-dependent and time-independent multi-orbital mean-fields for bosons.

#### IV. ILLUSTRATIVE NUMERICAL EXAMPLE

Having derived the time-dependent multi-orbital mean-field TDMF( $n$ ) we wish to apply it to a specific problem of evolution of fragmented condensates. Of course, we have to chose a specific shape for the interparticle interaction and we do so by taking the popular contact interaction,  $\lambda_0 V(\mathbf{r}_i - \mathbf{r}_j) = \lambda_0 \delta(\mathbf{r}_i - \mathbf{r}_j)$ , see Refs. [1,2]. The resulting set of  $n_{orb}$  equations (27) simplifies considerably and is given by,  $k = 1, \dots, n_{orb}$ :

$$i \dot{|\phi_k\rangle} = \mathbf{P} \left[ \hat{h} + \lambda_0(n_k - 1)|\phi_k|^2 + \sum_{l \neq k}^{n_{orb}} 2\lambda_0 n_l |\phi_l|^2 \right] |\phi_k\rangle, \\ \mathbf{P} = \left( 1 - \sum_{j=1}^{n_{orb}} |\phi_j\rangle \langle \phi_j| \right). \quad (28)$$

The factor of 2 in the last term of the square braces comes from the fact that *both* the exchange and direct potentials are now local potentials which are *equal* to one another, namely,  $\hat{J}_l(\mathbf{r}, t) = \hat{K}_l(\mathbf{r}, t) = |\phi_l(\mathbf{r}, t)|^2$ . Eq. (28) is the generalization of the time-dependent Gross-Pitaevskii equation (13) and will be applied below for a one-dimensional problem of a two-fold fragmented condensate evolving in time, i.e., for  $n_{orb} = 2$ .

As an illustrative numerical example we consider  $N = 1000$  interacting bosons in a double-well potential. The numerical implementation of TDMF(2) employs the discrete variable representation (DVR) method [23] and Adams-Bashforth-Moulton predictor-corrector integrator [24]. It is convenient to work in dimensionless units in which the one-body Hamiltonian reads  $\hat{h}(x) = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x)$ . As the trapping potential we chose the symmetric potential  $V(x) = 0.05x^2 + 10/\sqrt{2\pi}e^{-x^2/8}$ . The interparticle interaction strength is  $\lambda_0 = 0.1$ . Initially, the system is prepared in the symmetric double-well  $V(x)$  in a two-fold fragmented

(or, Fock) state  $\Phi = |n_1, n_2\rangle$ , with  $n_1 = n_2 = N/2$  bosons per fragment. The two orthonormal orbitals  $\phi_1(x, t = 0)$  and  $\phi_2(x, t = 0)$  in which the fragments initially reside are localized in the left and right wells of  $V(x)$ . At time  $t = 0$ , the symmetric potential trap  $V(x)$  is suddenly translated to  $V(x + 2)$  and the system is subsequently allowed to propagate in time in the new shifted potential  $V(x + 2)$  according to the TDMF equation (28). Since the system is not in a stationary state any more, the density

$$\rho(x, t) = \sum_k^{n_{orb}} n_k |\phi_k(x, t)|^2 = \frac{N}{2} [|\phi_1(x, t)|^2 + |\phi_2(x, t)|^2] \quad (29)$$

evolves in time.

In Fig. 1 we record four snapshots of the time-dependent density  $\rho(x, t)$ . As can be seen in the figure, the density profile as a whole oscillates from side to side, which is expected from this scenario where the trap has been shifted at  $t = 0$ . Atop this behavior of  $\rho(x, t)$ , we observe that the initial sharp dip of the fragmented-state density at  $t = 0$  nearly vanishes at  $t = 0.9$ , then it is restored at  $t = 5.5$ , and again it nearly vanishes at  $t = 6.7$ . Furthermore, a few density wiggles which vary in time accommodate  $\rho(x, t)$  in addition to the above features, all demonstrating that the time-evolution of fragmented condensates is both an intricate and appealing dynamical problem which awaits and invites ample investigations.

## V. SUMMARY

The evolution of Bose-Einstein condensates has been extensively studied by the well-known time-dependent Gross-Pitaevskii equation, which assumes all bosons to reside in the same time-dependent orbital. In this work we addressed the evolution of fragmented condensates, for which two (or more) orbitals are occupied, and derived a corresponding time-dependent multi-orbital mean-field theory, thus generalizing the (one-orbital) time-dependent Gross-Pitaevskii mean-field. We call our theory TDMF( $n$ ), where  $n = n_{orb}$  stands for the number of evolving fragments (orbitals).

In the TDMF, the ansatz for the many-body wavefunction is taken as a permanent made of  $n_{orb}$  time-dependent orthonormal orbitals, whose occupations are determined, say,

by the initial conditions. The evolution of the many-body wavefunction is then determined variationally by utilizing the usual functional action. This results in a set of  $n_{orb}$  coupled time-dependent equations for the evolution of the  $n_{orb}$  orbitals (fragments) in time. Working equations for a general two-body interaction between the bosons are explicitly presented. By considering their propagation in imaginary time, TDMF is shown to naturally relate to the recently developed and successfully employed *stationary* multi-orbital mean-field theory.

Finally, an illustrative numerical example of the evolution of a two-fold fragmented condensate in a one-dimensional double-well trap is provided, demonstrating an intricate dynamics of the density as time progresses. This is the tip of the iceberg of dynamical properties of fragmented Bose-Einstein condensates which await many more investigations.

#### ACKNOWLEDGMENTS

We thank Hans-Dieter Meyer for helpful discussions and making available the numerical integrator.

## REFERENCES

- [1] A. J. Leggett, Rev. Mod. Phys. **73**, 307 (2001).
- [2] L. Pitaevskii and S. Stringari, *Bose-Einstein Condensation* (Oxford University Press, Oxford, 2003).
- [3] L. D. Carr, Charles W. Clark, and W. P. Reinhardt, Phys. Rev. A **62**, 063610 (2000).
- [4] R. Baer, Phys. Rev. A **62**, 063810 (2000).
- [5] H. Saito and M. Ueda, Phys. Rev. Lett. **90**, 040403 (2003).
- [6] Z. X. Liang, Z. D. Zhang, and W. M. Liu, Phys. Rev. Lett. **94**, 050402 (2005).
- [7] S. Komineas and J. Brand, Phys. Rev. Lett. **95**, 110401 (2005).
- [8] L. Sanchez-Palencia and L. Santos, Phys. Rev. A **72**, 053607 (2005).
- [9] D. Ananikian and T. Bergeman, Phys. Rev. A, **73**, 013604 (2006).
- [10] L. S. Cederbaum and A. I. Streltsov, Phys. Lett. A **318**, 564 (2003); L. S. Cederbaum and A. I. Streltsov, Phys. Rev. A **70**, 023610 (2004).
- [11] O. E. Alon, A. I. Streltsov, and L. S. Cederbaum, Phys. Lett. A **347**, 88 (2005).
- [12] R. Kanamoto, H. Saito, and M. Ueda, Phys. Rev. A **67**, 013608 (2003).
- [13] D. Masiello, S. B. McKagan, and W. P. Reinhardt, Phys. Rev. A **72**, 063624 (2005).
- [14] E. J. Mueller, T.-L. Ho, M. Ueda, and G. Baym, cond-mat/0605711.
- [15] A. I. Streltsov, L. S. Cederbaum, and N. Moiseyev, Phys. Rev. A **70**, 053607 (2004).
- [16] A. I. Streltsov and L. S. Cederbaum, Phys. Rev. A **71**, 063612 (2005).
- [17] O. E. Alon, A. I. Streltsov, and L. S. Cederbaum, Phys. Rev. Lett **95**, 030405 (2005).
- [18] O. E. Alon and L. S. Cederbaum, Phys. Rev. Lett **95**, 140402 (2005).

- [19] P. Kramer and M. Saracento, *Geometry of the time-dependent variational principle* (Springer, Berlin, 1981).
- [20] H.-J. Kull and D. Pfirsch, Phys. Rev. E **61**, 5940 (2000).
- [21] A. I. Streltsov, O. E. Alon, and L. S. Cederbaum (unpublished).
- [22] H.-D. Meyer, U. Manthe, and L. S. Cederbaum, Chem. Phys. Lett. **165**, 73 (1990).
- [23] Z. Bačić and J. C. Light, J. Chem. Phys. **85**, 4594 (1986).
- [24] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in Fortran* (Cambridge Univ. Press, Cambridge, 1992), 2nd ed.

# FIGURES

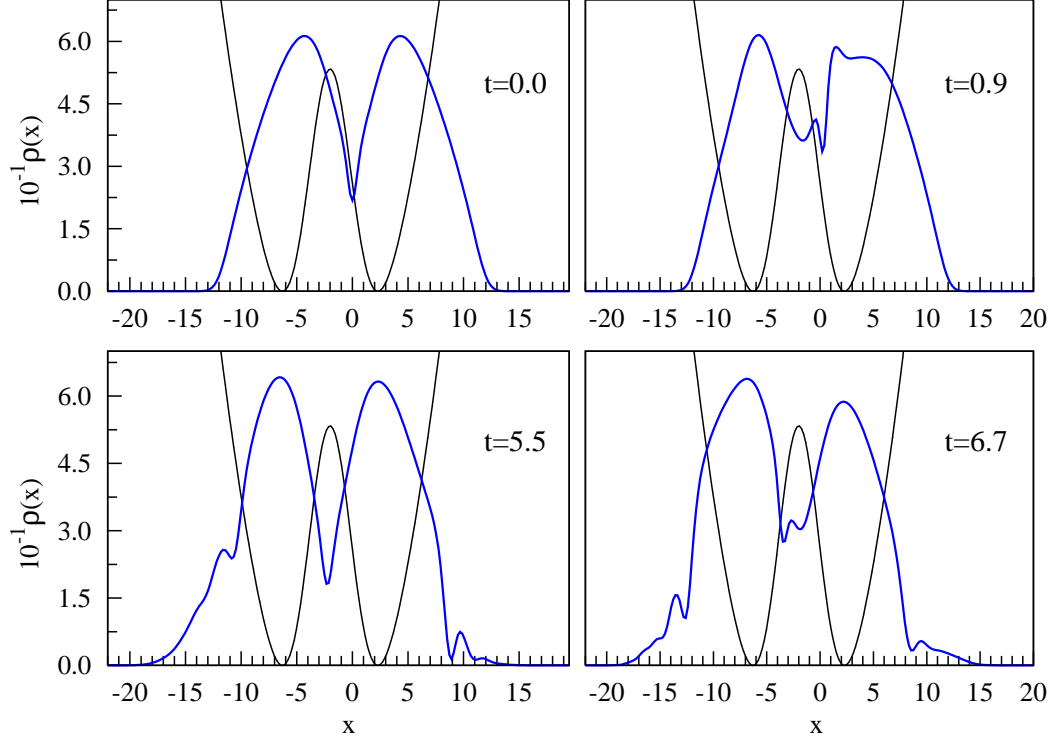


FIG. 1. (Color online) Time evolution of fragmented condensate made of  $N = 1000$  bosons in a double-well potential. A two-fold fragmented state  $\Phi = |N/2, N/2\rangle$  is initially prepared in a symmetric double-well trap  $V(x)$ . At time  $t = 0$ , the trap is suddenly translated a bit to the left, namely,  $V(x) \rightarrow V(x+2)$ , and the fragmented condensate is allowed to propagate in time according to the TDMF equation (28). Shown are four time snapshots of the density (blue curves), Eq. (29). It exhibits an intricate record of overall oscillations from side to side, evolution of the initial, central dip, and appearance of additional density wiggles which varies in time. For convenience, the trap potential  $V(x+2)$  (black curves) is shown, scaled by 2 and shifted vertically such that  $V = 0$  at its minima.